

Supplementary material to paper:

Revised molecular constants and term values for the X²Π state of CH.

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Part 1: Term values (cm⁻¹) of the v = 0–5 levels of the X²Π state of the CH radical.

**Part 2: Spectroscopic IR measurements (cm⁻¹) used in this work along with the
observed - calculated values obtained from the fit.**

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Part 1: Term values (cm⁻¹) of the v = 0–5 levels of the X²Π state of the CH radical.

J	v = 0				v = 1			
	F _{1e}	F _{1f}	F _{2e}	F _{2f}	F _{1e}	F _{1f}	F _{2e}	F _{2f}
0.5	-	-	14.2781	14.3900			2746.0998	2746.2069
1.5	32.1791	32.1566	81.2184	81.4642	2763.9482	2763.9285	2811.1644	2811.3979
2.5	87.5862	87.4260	167.4754	167.9694	2817.2855	2817.1324	2894.1910	2894.6636
3.5	172.0411	171.6676	281.1281	281.9447	2898.5811	2898.2219	3003.5854	3004.3688
4.5	284.9664	284.3047	422.5100	423.7223	3007.2778	3006.6403	3139.6652	3140.8298
5.5	426.0848	425.0612	591.5855	593.2651	3143.1058	3142.1190	3302.3921	3304.0069
6.5	595.1660	593.7089	788.2039	790.4199	3305.8400	3304.4348	3491.6166	3493.7481
7.5	791.9746	790.0142	1012.1526	1014.9717	3495.2490	3493.3584	3707.1286	3709.8412
8.5	1016.2538	1013.7229	1263.1739	1266.6601	3711.0806	3708.6399	3948.6743	3952.0294
9.5	1267.7196	1264.5539	1540.9723	1545.1863	3953.0554	3950.0028	4215.9624	4220.0185
10.5	1546.0592	1542.1972	1845.2174	1850.2167	4220.8656	4217.1420	4508.6675	4513.4797
11.5	1850.9299	1846.3136	2175.5465	2181.3849	4514.1737	4509.7235	4826.4321	4832.0522
12.5	2181.9592	2176.5341	2531.5659	2538.2935	4832.6129	4827.3839	5168.8683	5175.3441
13.5	2538.7456	2532.4608	2912.8522	2920.5152	5175.7876	5169.7311	5535.5588	5542.9345
14.5	2920.8587	2913.6672	3318.9538	3327.5943	5543.2736	5536.3449	5926.0582	5934.3738
15.5	3327.8407	3319.6995	3749.3916	3759.0478	5934.6195	5926.7777	6339.8938	6349.1854
16.5	3759.2069	3750.0769	4203.6607	4214.3664	6349.3471	6340.5554	6776.5674	6786.8669
17.5	4214.4469	4204.2933	4681.2313	4693.0162	6786.9528	6777.1783	7235.5556	7246.8910
18.5	4693.0259	4681.8178	5181.5499	5194.4399	7246.9082	7236.1224	7716.3117	7728.7066
19.5	5194.3857	5182.0963	5704.0409	5718.0577	7728.6619	7716.8399	8218.2665	8231.7407
20.5	5717.9463	5704.5526	6248.1079	6263.2695	8231.6402	8218.7613	8740.8296	8755.3992
21.5	6263.1069	6248.5896	6813.1347	6829.4557	8755.2486	8741.2957	9283.3909	9299.0682
22.5	6829.2478	6813.5910	7398.4872	7415.9790	9298.8728	9283.8325	9845.3215	9862.1155
23.5	7415.7312	7398.9224	8003.5149	8022.1857	9861.8807	9845.7427	10425.9756	10443.8924
24.5	8021.9036	8003.9328	8627.5518	8647.4078	10443.6230	10426.3802	11024.6915	11043.7343
25.5	8647.0965	8627.9563	9269.9189	9290.9640	11043.4352	11025.0831	11640.7930	11660.9630

26.5	9290.6288	9270.3136	9929.9250	9952.1618	11660.6389	11641.1750	12273.5909	12294.8876
27.5	9951.8078	9930.3135	10606.8687	10630.2992	12294.5433	12273.9668	12922.3847	12944.8063
28.5	10629.9315	10607.2543	11300.0400	11324.6661	12944.4466	12922.7577	13586.4636	13610.0082
29.5	11324.2899	11300.4262	12008.7221	12034.5464	13609.6375	13586.8369	14265.1083	14289.7740
30.5	12034.1667	12009.1122	12732.1928	12759.2198	14289.3972	14265.4851	14957.5923	14983.3784
31.5	12758.8418	12732.5901	13469.7265	13497.9632	14983.0001	14957.9757	15663.1834	15690.0914
32.5	13497.5922	13470.1343	14220.5961	14250.0533	15689.7163	15663.5766	16381.1453	16409.1795
33.5	14249.6943	14221.0176	14984.0740	15014.7674	16408.8124	16381.5514	17110.7388	17139.9077
34.5	15014.4260	14984.5126	15759.4349	15791.3864	17139.5534	17111.1609	17851.2235	17881.5408
35.5	15791.0678	15759.8938	16545.9567	16579.1956	17881.2042	17851.6647	18601.8590	18633.3449
36.5	16578.9053	16546.4393	17342.9227	17377.4874	18633.0309	18602.3224	19361.9064	19394.5888
37.5	17377.2309	17343.4323	18149.6232	18185.5625	19394.3025	19362.3952	20130.6294	20164.5458
38.5	18185.3455	18150.1631	18965.3571	19002.7322	20164.2922	20131.1468	20907.2962	20942.4947
39.5	19002.5604	18965.9308	19789.4341	19828.3199	20942.2790	20907.8454	21691.1800	21727.7213

J	v = 2				v = 3			
	F_{1e}	F_{1f}	F_{2e}	F_{2f}	F_{1e}	F_{1f}	F_{2e}	F_{2f}
0.5			5351.8335	5351.9364			7833.0285	7833.1272
1.5	5369.6551	5369.6391	5415.1039	5415.3253	7850.7428	7850.7302	7894.4704	7894.6800
2.5	5420.9479	5420.8031	5494.9201	5495.3721	7900.0113	7899.8744	7971.0922	7971.5235
3.5	5499.1146	5498.7711	5600.0897	5600.8411	7975.0729	7974.7447	8072.0629	8072.7820
4.5	5603.6208	5603.0090	5730.9108	5732.0293	8075.4179	8074.8317	8197.6591	8198.7311
5.5	5734.2048	5733.2565	5887.3418	5888.8937	8200.7934	8199.8835	8347.8347	8349.3233
6.5	5890.6464	5889.2951	6069.2335	6071.2831	8350.9841	8349.6866	8522.4405	8524.4074
7.5	6072.7186	6070.8999	6276.3784	6278.9873	8525.7670	8524.0200	8721.2707	8723.7752
8.5	6280.1733	6277.8249	6508.5258	6511.7532	8724.8977	8722.6415	8944.0774	8947.1763
9.5	6512.7354	6509.7980	6765.3883	6769.2904	8948.1051	8945.2827	9190.5765	9194.3237
10.5	6770.1018	6766.5187	7046.6450	7051.2746	9195.0900	9191.6471	9460.4509	9464.8970
11.5	7051.9397	7047.6577	7351.9433	7357.3499	9465.5242	9461.4097	9753.3520	9758.5445
12.5	7357.8878	7352.8567	7680.9003	7687.1299	9759.0506	9754.2167	10068.9015	10074.8842
13.5	7687.5556	7681.7290	8033.1043	8040.1988	10075.2836	10069.6859	10406.6921	10413.5053
14.5	8040.5247	8033.8601	8408.1155	8416.1131	10413.8095	10407.4074	10766.2887	10773.9686
15.5	8416.3495	8408.8080	8805.4670	8814.4019	10774.1876	10766.9442	11147.2293	11155.8083
16.5	8814.5578	8806.1045	9224.6664	9234.5687	11155.9505	11147.8327	11549.0259	11558.5324
17.5	9234.6517	9225.2559	9665.1962	9676.0918	11558.6052	11549.5841	11971.1656	11981.6240
18.5	9676.1089	9665.7437	10126.5152	10138.4262	11981.6338	11971.6844	12413.1115	12424.5421

19.5	10138.3835	10127.0263	10608.0598	10621.0040	12424.4949	12413.5961	12874.3035	12886.7227
20.5	10620.9074	10608.5393	11109.2446	11123.2362	12886.6239	12874.7586	13354.1597	13367.5800
21.5	11123.0910	11109.6969	11629.4639	11644.5135	13367.4347	13354.5896	13852.0769	13866.5072
22.5	11644.3247	11629.8932	12168.0931	12184.2076	13866.3202	13852.4856	14367.4319	14382.8775
23.5	12183.9800	12168.5031	12724.4893	12741.6726	14382.6534	14367.8232	14899.5826	14916.0455
24.5	12741.4110	12724.8837	13297.9930	13316.2462	14915.7887	14899.9600	15447.8687	15465.3480
25.5	13315.9550	13298.3752	13887.9289	13907.2508	15465.0628	15448.2354	16011.6125	16030.1048
26.5	13906.9345	13888.3024	14493.6078	14513.9950	16029.7954	16011.9719	16590.1206	16609.6203
27.5	14513.6579	14493.9756	15114.3268	15135.7747	16609.2907	16590.4757	17182.6839	17203.1836
28.5	15135.4212	15114.6921	15749.3714	15771.8746	17202.8381	17183.0379	17788.5792	17810.0705
29.5	15771.5089	15749.7372	16398.0161	16421.5691	17809.7131	17788.9350	18407.0695	18429.5435
30.5	16421.1957	16398.3855	17059.5261	17084.1240	18429.1783	18407.4301	19037.4051	19060.8531
31.5	17083.7471	17059.9020	17733.1578	17758.7973	19060.4840	19037.7734	19678.8243	19703.2383

J	v = 4				v = 5			
	F_{1e}	F_{1f}	F_{2e}	F_{2f}	F_{1e}	F_{1f}	F_{2e}	F_{2f}
0.5			10190.6695	10190.7642			12425.3197	12425.4099
1.5	10208.2778	10208.2691	10250.3370	10250.5347	12442.7955	12442.7903	12483.2364	12483.4216
2.5	10255.5386	10255.4101	10323.7664	10324.1773	12488.0594	12487.9392	12553.4662	12553.8557
3.5	10327.5102	10327.1978	10420.5490	10421.2362	12556.9471	12556.6504	12646.0586	12646.7127
4.5	10423.7112	10423.1509	10540.9358	10541.9620	12649.0083	12648.4739	12761.2349	12762.2134
5.5	10543.8978	10543.0265	10684.8751	10686.3014	12764.0085	12763.1761	12898.9362	12900.2976
6.5	10687.8596	10686.6160	10852.2172	10854.1026	12901.7420	12900.5528	13059.0104	13060.8114
7.5	10855.3774	10853.7021	11042.7572	11045.1588	13061.9924	13060.3896	13241.2526	13243.5477
8.5	11046.2102	11044.0459	11256.2493	11259.2215	13244.5211	13242.4499	13445.4178	13448.2591
9.5	11260.0903	11257.3823	11492.4119	11496.0063	13449.0627	13446.4707	13671.2255	13674.6623
10.5	11496.7219	11493.4183	11750.9309	11755.1961	13675.3234	13672.1611	13918.3631	13922.4419
11.5	11755.7803	11751.8321	12031.4611	12036.4422	13922.9807	13919.2012	14186.4868	14191.2508
23.5	16457.7968	16443.6187	16951.0411	16966.7680				
24.5	16966.5052	16951.3844	17473.9529	17490.6362				
25.5	17490.3446	17474.2844	18011.3117	18028.9441				
26.5	18028.6275	18011.6344	18562.4149	18580.9865				
27.5	18580.6487	18562.7315	19126.5421	19146.0407				

Part 2: Spectroscopic measurements (cm^{-1}) used in this work along with the observed-calculated values obtained from the fits.

1-0	J	ν (cm^{-1})	$o - c$
P_{1ee}	2.5	2676.3596	-0.0025
	3.5	2645.2425	-0.0018
	4.5	2613.6122	-0.0025
	5.5	2581.1915	-0.0015
	6.5	2547.9392	-0.0006
	7.5	2513.8620	-0.0033
	8.5	2478.9750	-0.0200
	9.5	2443.3550	-0.0060
	10.5	2406.9950	-0.0012
	11.5	2369.9280	-0.0077
	12.5	2332.2100	-0.0045
	13.5	-	
	14.5	2254.9070	-0.0220
	15.5	2215.4320	-0.0009
16.5	2175.4230	0.0104	
17.5	2134.8750	-0.0250	
18.5	2093.9330	0.0061	
P_{1ff}	2.5	2676.5015	-0.0010
	3.5	2645.4638	-0.0010
	4.5	2613.9174	0.0002
	5.5	2581.5800	0.0010
	6.5	2548.4114	0.0012
	7.5	2514.4203	-0.0003
	8.5	2479.6357	0.0002

P_{2ee}	9.5	2444.0792	-0.0068
	10.5	2407.8050	-0.0005
	11.5	2370.8350	0.0066
	12.5	2333.2050	0.0160
	13.5	2294.9220	-0.0011
	14.5	2256.0560	-0.0079
	15.5	2216.6490	0.0036
	16.5	2176.7500	0.0490
	17.5	2136.2660	0.0039
	1.5	2664.8854	0.0040
	2.5	2643.6918	0.0028
	3.5	2613.0658	0.0029
	4.5	2581.0761	0.0006
	5.5	2548.0781	-0.0016
	6.5	2514.1902	0.0020
	7.5	2479.4701	0.0062
	8.5	2443.9566	0.0020
9.5	2407.7150	0.0130	
10.5	2370.7550	0.0100	
11.5	2333.1300	0.0090	
12.5	2294.8570	-0.0092	
13.5	2255.9810	-0.0350	
14.5	2216.5970	-0.0081	
15.5	2176.6880	0.0214	
P_{2ff}	1.5	2664.7423	-0.0004
	2.5	2643.4318	0.0034
	3.5	2612.7230	0.0041
	4.5	2580.6503	0.0038
	5.5	2547.5685	0.0037
	6.5	2513.5906	0.0036
	7.5	2478.7794	0.0030
	8.5	2443.1844	0.0033
	9.5	2406.8450	0.0019
	10.5	2369.8150	0.0132
	11.5	2332.0760	0.0020

	12.5	2293.7490	-0.0097
	13.5	2254.8090	-0.0199
	14.5	2215.3470	0.0069
	15.5	2175.3240	-0.0020
	16.5	2134.8040	-0.0151
Q_{1fe}	1.5	2731.7481	-0.0013
	2.5	2729.5440	-0.0023
	3.5	2726.1720	-0.0088
	4.5	2721.6600	-0.0138
	5.5	2716.0370	0.0027
	6.5	2709.2640	-0.0048
	7.5	2701.3940	0.0102
Q_{1ef}	1.5	2731.7920	0.0004
	2.5	2729.8587	-0.0008
	3.5	2726.9150	0.0020
	4.5	2722.9750	0.0019
	5.5	2718.0470	0.0024
	6.5	2712.1320	0.0009
	7.5	2705.2250	-0.0098
Q_{2fe}	1.5	2730.1768	-0.0027
	2.5	2727.1860	-0.0022
	3.5	2723.2410	0.0003
	4.5	2718.3220	0.0021
	5.5	2712.4200	-0.0014
	6.5	2705.5420	-0.0022
Q_{2ef}	1.5	2729.7021	0.0019
	2.5	2726.2210	-0.0005
	3.5	2721.6300	-0.0108
	4.5	2715.9440	0.0011
	5.5	2709.1300	0.0029
	6.5	2701.2010	0.0044
R_{1ee}	1.5	2785.1080	0.0017
	2.5	2810.9964	0.0014
	3.5	2835.2362	-0.0005
	4.5	2858.1400	0.0006

	5.5	2879.7533	-0.0019
	6.5	2900.0841	0.0011
	7.5	2919.1025	-0.0034
	8.5	2936.8003	-0.0014
	9.5	2953.1449	-0.0011
	10.5	2968.1110	-0.0035
	11.5	2981.6810	-0.0021
	12.5	2993.8220	-0.0064
	13.5	3004.5210	-0.0071
	14.5	3013.7600	-0.0008
	15.5	3021.5070	0.0006
	16.5	3027.7440	-0.0019
	17.5	3032.4590	-0.0023
	18.5	3035.6350	-0.0011
	19.5	3037.2520	-0.0026
	20.5	3037.3020	-0.0003
	21.5	3035.7720	0.0061
	22.5	3032.6370	0.0041
	23.5	3027.8970	0.0053
	24.5	3021.5320	0.0004
	25.5	3013.5610	0.0186
	26.5	3003.9010	-0.0135
	27.5	2992.6350	-0.0037
	28.5	2979.7010	-0.0050
	29.5	2965.1060	-0.0013
	30.5	2948.8250	-0.0084
	31.5	2930.8760	0.0015
	32.5	2911.2270	0.0067
	33.5	2889.8590	-0.0001
	34.5	2866.7720	-0.0062
	35.5	-	
	36.5	2815.4050	0.0078
	37.5	2787.0540	-0.0073
R_{1ff}	1.5	2784.9787	0.0029
	2.5	2810.7981	0.0022
	3.5	2834.9739	0.0013

	4.5	2857.8135	-0.0008
	5.5	2879.3743	0.0007
	6.5	2899.6514	0.0019
	7.5	2918.6245	-0.0012
	8.5	2936.2795	-0.0004
	9.5	2952.5852	-0.0030
	10.5	2967.5230	-0.0033
	11.5	2981.0660	-0.0043
	12.5	2993.1930	-0.0040
	13.5	3003.8847	0.0006
	14.5	3013.1060	-0.0045
	15.5	3020.8520	-0.0039
	16.5	3027.0990	-0.0024
	17.5	3031.8250	-0.0041
	18.5	3035.0140	-0.0081
	19.5	3036.6620	-0.0030
	20.5	3036.7500	0.0069
	21.5	3035.2420	-0.0009
	22.5	3032.1620	0.0103
	23.5	3027.4550	-0.0029
	24.5	3021.1470	-0.0033
	25.5	3013.2260	0.0073
	26.5	3003.6610	0.0078
	27.5	2992.4480	0.0038
	28.5	2979.5840	0.0014
	29.5	2965.0810	0.0221
	30.5	2948.8650	0.0014
	31.5	2930.9860	-0.0005
	32.5	2911.4120	-0.0051
	33.5	2890.1460	0.0027
	34.5	2867.1500	-0.0021
	35.5	2842.4270	-0.0016
	36.5	2815.9530	-0.0029
	37.5	2787.7130	-0.0016
	38.5	2757.6710	-0.0113
R_{2ee}	0.5	2796.8826	-0.0037
	1.5	2812.9725	-0.0001
	2.5	2836.1105	0.0005

3.5	2858.5391	0.0020
4.5	2879.8823	0.0002
5.5	2900.0336	0.0026
5.5	2900.0336	0.0026
6.5	2918.9274	0.0028
7.5	2936.5215	-0.0002
8.5	2952.7871	-0.0013
9.5	2967.6990	0.0038
10.5	2981.2110	-0.0037
11.5	2993.3230	0.0012
12.5	3003.9900	-0.0030
13.5	3013.2050	-0.0010
14.5	3020.9420	0.0019
15.5	3027.1740	-0.0018
16.5	3031.8950	0.0001
17.5	3035.0840	0.0036
18.5	3036.7231	0.0065
19.5	3036.7920	0.0033
20.5	3035.2820	-0.0010
21.5	3032.1820	-0.0049
22.5	3027.4800	-0.0084
23.5	3021.1770	0.0004
24.5	3013.2360	-0.0051
25.5	3003.6710	-0.0010
26.5	2992.4580	-0.0017
27.5	2979.5990	0.0041
28.5	2965.0810	0.0127
29.5	2948.8630	-0.0072
30.5	2930.9860	-0.0046
31.5	2911.4120	-0.0067
32.5	2890.1460	0.0032
33.5	2867.1500	0.0005
34.5	2842.4582	0.0341
35.5	2815.9540	0.0044
36.5	2787.7130	0.0063
37.5	2757.6710	-0.0020

R_{2ff}	0.5	2797.0075	-0.0004
	1.5	2813.2007	0.0013
	2.5	2836.4004	0.0010
	3.5	2858.8868	0.0016
	4.5	2880.2812	-0.0034
	5.5	2900.4867	0.0036
	6.5	2919.4172	-0.0041
	7.5	2937.0572	-0.0005
	8.5	2953.3629	0.0045
	9.5	2968.2910	-0.0024
	10.5	2981.8360	0.0005
	11.5	2993.9710	0.0117
	12.5	3004.6450	0.0040
	13.5	3013.8540	-0.0046
	14.5	3021.5920	0.0009
	15.5	3027.8240	0.0048
	16.5	3032.5270	0.0024
	17.5	3035.6880	-0.0024
	18.5	3037.3020	0.0011
	19.5	3037.3420	0.0005
	20.5	3035.7920	-0.0066
	21.5	3032.6570	-0.0028
	22.5	3027.9070	-0.0064
	23.5	3021.5620	0.0134
	24.5	3013.5710	0.0158
	25.5	3003.9110	-0.0126
	26.5	2992.6450	0.0005
	27.5	2979.7010	-0.0080
	28.5	2965.1060	-0.0019
	29.5	2948.8250	-0.0070
	30.5	2930.8760	0.0044
	31.5	2911.2270	0.0107
	32.5	2889.8590	0.0045
	33.5	2866.7720	-0.0014
	34.5	2841.9540	-0.0045
	35.5	2815.4030	0.0098
	36.5	2787.0540	-0.0045

2-1	J	ν (cm-1)	$o - c$
P_{1ee}	2.5	2552.3696	0.0000
	3.5	2522.3654	-0.0014
	4.5	2491.8350	-0.0018
	5.5	2460.5151	0.0001
	6.5	2428.3636	-0.0012
	7.5	2395.3990	0.0017
	8.5	2361.6400	0.0020
	9.5	-	
	10.5	2291.8680	-0.0018
	11.5	2255.9250	-0.0031
P_{1ff}	2.5	2552.5111	0.0044
	3.5	2522.5830	0.0018
	4.5	2492.1342	0.0034
	5.5	2460.8892	-0.0008
	6.5	2428.8256	0.0039
	7.5	2395.9405	0.0038
	8.5	2362.2550	-0.0050
	9.5	-	
	10.5	2292.6550	-0.0010
	11.5	2256.7990	0.0038
P_{2ee}	12.5	2220.2750	0.0012
	1.5	2540.7135	-0.0556
	2.5	2520.9132	0.0003
	3.5	2491.3354	0.0007
	4.5	2460.4291	0.0046
	5.5	2428.5202	0.0015
	6.5	2395.7268	0.0016
	7.5	2362.1000	-0.0049
	8.5	-	
	9.5	2292.5620	-0.0014
P_{2ff}	10.5	2256.7210	0.0001
	11.5	2220.2100	-0.0029
	1.5	2540.5856	-0.0471
	2.5	2520.6614	-0.0003
	3.5	2491.0104	0.0071
4.5	2460.0104	-0.0008	

	5.5	2428.0278	0.0053
	6.5	2395.1475	0.0019
	7.5	2361.4350	-0.0069
	8.5	-	
	9.5	2291.7370	0.0023
	10.5	2255.8030	-0.0076
Q_{1fe}	1.5	2605.6851	-0.0058
	2.5	2603.5180	0.0004
	3.5	2600.1858	-0.0042
	4.5	2595.7250	-0.0062
Q_{1ef}	1.5	2605.7252	-0.0013
	2.5	2603.8145	-0.0010
	3.5	2600.8970	0.0043
	4.5	2596.9840	0.0035
Q_{2fe}	0.5	2605.8820	-0.0454
	1.5	2604.1527	-0.0082
	2.5	2601.1780	-0.0032
	3.5	2597.2390	-0.0166
	4.5	2592.3700	0.0059
Q_{2ef}	0.5	2605.6856	-0.0590
	1.5	2603.7072	0.0012
	2.5	2600.2499	-0.0066
	3.5	2595.7225	0.0016
R_{1ee}	1.5	2657.0034	0.0037
	2.5	2681.8355	0.0063
	3.5	2705.0420	0.0023
	4.5	2726.9276	0.0006
	5.5	2747.5444	0.0039
	6.5	2766.8852	0.0065
	7.5	2784.9221	-0.0021
	8.5	2801.6559	0.0011
	9.5	2817.0445	-0.0018
	10.5	2831.0690	-0.0051
	11.5	2843.7120	-0.0021
	12.5	2854.9400	-0.0026
	13.5	2864.7360	-0.0011
	14.5	2873.0680	-0.0079
	15.5	2879.9340	-0.0043

R_{1ff}

16.5	2885.3040	-0.0005
17.5	2889.1540	-0.0021
18.5	2891.4630	-0.0123
19.5	2892.2450	-0.0004
20.5	2891.4630	0.0123
21.5	2889.0640	-0.0121
22.5	2885.1120	0.0048
23.5	2879.5400	0.0097
24.5	2872.3380	0.0060
25.5	2863.4930	-0.0063
26.5	2853.0370	0.0180
27.5	2840.8930	0.0151
28.5	2827.0640	0.0016
29.5	2811.5550	-0.0032
30.5	2794.3460	-0.0039
31.5	2775.4150	-0.0061
32.5	2754.7560	0.0028
33.5	2732.3300	0.0039
34.5	2708.1030	-0.0135
1.5	2656.8763	0.0017
2.5	2681.6406	0.0019
3.5	2704.7887	0.0016
4.5	2726.6191	0.0028
5.5	2747.1780	0.0019
6.5	2766.4658	0.0007
7.5	2784.4666	0.0001
8.5	2801.1534	-0.0047
9.5	2816.5168	0.0009
10.5	2830.5090	-0.0066
11.5	2843.1270	-0.0062
12.5	2854.3420	-0.0031
13.5	2864.1230	-0.0060
14.5	2872.4630	-0.0001
15.5	2879.3280	0.0012
16.5	2884.7140	0.0135
17.5	2888.5740	0.0086
18.5	2890.9170	0.0130
19.5	2891.6930	-0.0063

R_{2ee}

20.5	2890.9170	-0.0186
21.5	2888.5840	-0.0135
22.5	2884.6730	0.0024
23.5	2879.1470	0.0060
24.5	2871.9950	0.0000
25.5	2863.2180	-0.0013
26.5	2852.8020	0.0014
27.5	2840.7230	-0.0023
28.5	2826.9820	0.0025
29.5	2811.5480	-0.0006
30.5	2794.4148	-0.0021
31.5	2775.5660	-0.0015
32.5	2754.9850	0.0034
33.5	2732.6350	-0.0036
34.5	2708.5310	0.0160
35.5	2682.5700	-0.0145
36.5	2654.8180	0.0007
0.5	2669.0013	-0.0028
1.5	2683.7552	-0.0005
2.5	2705.8993	0.0005
3.5	2727.3235	-0.0019
4.5	2747.6770	0.0004
5.5	2766.8376	-0.0038
6.5	2784.7635	0.0016
7.5	2801.3970	-0.0002
8.5	2816.7159	0.0019
9.5	2830.6830	0.0004
10.5	2843.2770	0.0012
11.5	2854.4720	0.0038
12.5	2864.2430	0.0070
13.5	2872.5620	0.0054
14.5	2879.4030	-0.0058
15.5	2884.7740	0.0014
16.5	2888.6340	0.0052
17.5	2890.9730	0.0134
18.5	2891.7480	-0.0001
19.5	2890.9730	-0.0050
20.5	2888.6340	-0.0003

R_{2ff}

21.5	2884.6980	-0.0042
22.5	2879.1700	0.0022
23.5	2872.0130	-0.0043
24.5	2863.2380	0.0006
25.5	2852.8170	0.0022
26.5	2840.7330	-0.0029
27.5	2826.9820	-0.0046
28.5	2811.5550	0.0025
29.5	2794.4148	-0.0030
30.5	2775.5660	0.0005
31.5	2754.9850	0.0080
32.5	2732.6350	0.0035
33.5	2708.5310	0.0255
34.5	2682.5700	-0.0029
0.5	2669.1199	0.0015
1.5	2683.9733	-0.0010
2.5	2706.1774	-0.0001
3.5	2727.6604	-0.0001
4.5	2748.0685	0.0046
5.5	2767.2767	0.0005
6.5	2785.2421	0.0029
7.5	2801.9126	0.0006
8.5	2817.2660	0.0051
9.5	2831.2570	0.0009
10.5	2843.8720	0.0018
11.5	2855.0820	0.0043
12.5	2864.8570	0.0023
13.5	2873.1830	0.0044
14.5	2880.0280	-0.0001
15.5	2885.3900	0.0068
16.5	2889.2310	0.0061
17.5	2891.5200	-0.0152
18.5	2892.2970	-0.0004
19.5	2891.5200	0.0245
20.5	2889.1540	0.0397
21.5	2885.1360	-0.0035
22.5	2879.5550	-0.0021
23.5	2872.3530	-0.0008

	24.5	2863.5130	-0.0035
	25.5	2853.0370	0.0050
	26.5	2840.8830	-0.0042
	27.5	2827.0640	-0.0043
	28.5	2811.5550	-0.0060
	29.5	2794.3460	-0.0041
	30.5	2775.4150	-0.0038
	31.5	2754.7560	0.0070
	32.5	2732.3300	0.0099
	33.5	2708.1030	-0.0063
	34.5	2682.0930	0.0026
	35.5	2654.2890	0.0548
	36.5	2624.5120	0.0053
3-2	J	ν (cm-1)	o - c
P_{1ee}	2.5	2429.7957	0.0008
	3.5	2400.8980	0.0013
	4.5	2371.4430	-0.0091
	5.5	2341.2130	-0.0002
	6.5	2310.1480	0.0009
	7.5	2278.2660	0.0005
	8.5	2245.5950	0.0012
P_{1ff}	2.5	2429.9281	0.0010
	3.5	2401.1078	0.0045
	4.5	2371.7354	-0.0003
	5.5	2341.5724	-0.0027
	6.5	2310.5873	-0.0011
	7.5	2278.7960	0.0093
	8.5	2246.2160	0.0209
P_{2ee}	2.5	2399.5608	0.0105
	3.5	2371.0052	0.0028
	4.5	2341.1533	0.0012
	5.5	2310.3176	0.0003
	6.5	2278.5960	-0.0052
	7.5	2246.0640	0.0019
P_{2ff}	2.5	2399.3112	0.0033
	3.5	2370.6852	0.0028
	4.5	2340.7578	0.0051

	5.5	2309.8392	0.0018
	6.5	2278.0410	0.0008
	7.5	2245.4200	0.0000
Q_{1fe}	1.5	2481.0780	0.0028
	2.5	2478.9210	-0.0056
	3.5	2475.6270	-0.0030
	4.5	2471.2050	-0.0059
	5.5	2465.6794	0.0006
Q_{1ef}	1.5	2481.0966	-0.0071
	2.5	2479.2100	0.0018
	3.5	-	
	4.5	2472.4030	-0.0059
	5.5	2467.5357	-0.0012
	6.5	2461.6740	-0.0150
	7.5	2454.8670	-0.0001
Q_{2fe}	1.5	2479.5758	-0.0003
	2.5	-	
	3.5	2472.7060	0.0137
	4.5	2467.8212	0.0009
	5.5	2461.9730	-0.0085
	6.5	2455.1660	-0.0079
Q_{2ef}	1.5	2479.1403	-0.0048
	2.5	2475.7210	0.0010
	3.5	2471.2050	-0.0169
	4.5	2465.6200	-0.0098
	5.5	2458.9400	-0.0010
	6.5	2451.1560	-0.0015
R_{1ee}	1.5	2530.3620	0.0058
	2.5	-	
	3.5	2576.3047	0.0014
	4.5	2597.1737	0.0010
	5.5	2616.7795	0.0001
	6.5	2635.1161	-0.0046
	7.5	2652.1827	0.0037
	8.5	2667.9333	0.0015
	9.5	2682.3550	0.0004
	10.5	2695.4260	0.0036
	11.5	2707.1120	0.0011

R_{1ff}

12.5	2717.3980	0.0022
13.5	2726.2520	-0.0020
14.5	2733.6632	0.0003
15.5	2739.6010	0.0000
16.5	2744.0470	-0.0004
17.5	2746.9800	-0.0021
18.5	2748.3860	0.0000
19.5	2748.2430	0.0026
20.5	2746.5220	-0.0054
21.5	2743.2300	0.0008
22.5	2738.3400	0.0113
23.5	2731.8120	0.0033
24.5	2723.6530	0.0012
25.5	2713.8360	-0.0044
26.5	2702.3520	-0.0043
27.5	2689.1810	0.0007
28.5	2674.2940	0.0021
29.5	2657.6750	0.0057
30.5	2639.2890	0.0006
31.5	2619.1120	-0.0105
1.5	2530.2379	0.0026
2.5	2553.9456	0.0040
3.5	2576.0652	0.0046
4.5	2596.8775	0.0030
5.5	2616.4308	0.0007
6.5	2634.7270	0.0021
7.5	2651.7420	0.0004
8.5	2667.4550	-0.0028
9.5	2681.8420	-0.0071
10.5	2694.8910	0.0000
11.5	2706.5610	0.0020
12.5	2716.8300	0.0008
13.5	2725.6760	-0.0024
14.5	2733.0870	0.0029
15.5	2739.0230	-0.0017
16.5	2743.4780	-0.0016
17.5	2746.4290	0.0005
18.5	2747.8460	-0.0063

R_{2ee}

19.5	2747.7320	-0.0003
20.5	2746.0550	0.0046
21.5	2742.7880	-0.0008
22.5	2737.9350	0.0050
23.5	2731.4600	0.0032
24.5	2723.3460	-0.0057
25.5	2713.6000	0.0034
26.5	2702.1850	0.0117
27.5	2689.0610	-0.0013
28.5	2674.2400	-0.0029
29.5	2657.6900	-0.0029
30.5	2639.3850	-0.0029
31.5	2619.3040	0.0028
1.5	2555.9899	0.0016
2.5	2577.1414	-0.0014
3.5	2597.5711	0.0017
4.5	2616.9257	0.0018
5.5	2635.0898	-0.0089
6.5	2652.0381	0.0009
7.5	2667.6995	0.0005
8.5	2682.0500	-0.0007
9.5	2695.0590	-0.0036
10.5	2706.7030	-0.0040
11.5	2716.9520	-0.0062
12.5	2725.7930	0.0012
13.5	2733.1870	0.0026
14.5	2739.1130	-0.0008
15.5	2743.5570	-0.0019
16.5	2746.5090	0.0098
17.5	2747.9180	0.0027
18.5	2747.7870	-0.0013
19.5	2746.1060	0.0061
20.5	2742.8280	-0.0043
21.5	2737.9600	-0.0080
22.5	2731.4800	-0.0095
23.5	2723.3800	0.0006
24.5	2713.6200	0.0004
25.5	2702.1950	0.0034

	26.5	2689.0710	-0.0051
	27.5	2674.2500	-0.0024
	28.5	2657.6900	-0.0081
	29.5	2639.3850	-0.0040
	30.5	2619.3040	0.0058
R_{2ff}	1.5	2556.1929	-0.0053
	2.5	2577.4096	-0.0003
	3.5	2597.8929	0.0028
	4.5	2617.2953	0.0014
	5.5	2635.5158	0.0021
	6.5	2652.4956	0.0034
	7.5	2668.1862	-0.0028
	8.5	2682.5770	0.0066
	9.5	2695.6030	-0.0036
	10.5	2707.2680	-0.0019
	11.5	2717.5400	0.0057
	12.5	2726.3760	0.0006
	13.5	2733.7690	-0.0008
	14.5	2739.6960	0.0008
	15.5	2744.1270	-0.0035
	16.5	2747.0570	0.0017
	17.5	2748.4550	0.0047
	18.5	2748.2970	0.0005
	19.5	2746.5680	-0.0080
	20.5	2743.2710	0.0001
	21.5	2738.3670	0.0030
	22.5	2731.8270	-0.0109
	23.5	2723.6730	-0.0024
	24.5	2713.8560	-0.0026
	25.5	2702.3660	-0.0035
	26.5	2689.1910	0.0023
	27.5	2674.2940	-0.0018
	28.5	2657.6750	0.0061
	29.5	2639.2890	0.0051
	30.5	2619.1120	-0.0022
4-3	J	v (cm-1)	o - c
P_{1ee}	2.5	2308.2669	0.0004

	3.5	2280.4625	-0.0032
	4.5	2252.0956	0.0034
	5.5	2222.9080	-0.0098
	6.5	2192.9111	-0.0026
	7.5	2162.0916	-0.0010
	8.5	2130.4830	0.0032
	9.5	2098.1043	-0.0008
P_{1ff}	2.5	2308.3953	0.0007
	3.5	2280.6694	0.0040
	4.5	2252.3615	-0.0046
	5.5	2223.2650	-0.0023
	6.5	2193.3480	0.0081
	7.5	2162.5969	0.0009
	8.5	2131.0610	0.0004
	9.5	2098.7653	0.0021
P_{2ee}	1.5	2296.2426	0.0435
	2.5	2279.2365	-0.0084
	3.5	2251.7012	-0.0022
	4.5	2222.9080	0.0181
	5.5	2193.1051	0.0040
	6.5	2162.4210	-0.0136
	7.5	2130.9390	-0.0074
	8.5	2098.6799	0.0001
P_{2ff}	2.5	2279.0668	0.0556
	3.5	2251.3920	-0.0033
	4.5	2222.5051	0.0000
	5.5	2192.6392	0.0005
	6.5	2161.8770	-0.0170
	7.5	2130.3230	-0.0044
	8.5	2097.9828	0.0003
Q_{1fe}	1.5	2357.5285	0.0022
	2.5	2355.4080	0.0092
	3.5	2352.1210	-0.0039
Q_{1ef}	1.5	2357.5453	-0.0023
	2.5	2355.6663	0.0022
	3.5	2352.7701	0.0046
Q_{2fe}	1.5	2356.0638	-0.0004
	2.5	2353.0910	0.0059

Q_{2ef}	1.5	2355.6663	0.0093
	2.5	2352.2462	0.0033
R_{1ee}	1.5	2404.7967	0.0009
	2.5	2427.4996	0.0007
	3.5	2448.6388	0.0004
	4.5	2468.4795	-0.0004
	5.5	2487.0703	0.0041
	6.5	2504.3913	-0.0020
	7.5	2520.4424	-0.0007
	8.5	2535.1936	0.0010
	9.5	2548.6110	-0.0058
	10.5	2560.6850	-0.0053
	11.5	2571.3860	-0.0017
	12.5	-	
	13.5	2588.5531	-0.0021
	14.5	2594.9920	0.0149
	15.5	2599.9310	0.0046
	16.5	2603.3760	-0.0045
	17.5	2605.3100	-0.0071
	18.5	2605.7150	0.0008
	19.5	2604.5620	0.0117
	20.5	2601.8020	-0.0018
21.5	2597.4470	-0.0062	
22.5	2591.4780	0.0014	
23.5	2583.8460	-0.0058	
24.5	2574.5510	-0.0048	
25.5	2563.5610	-0.0037	
26.5	2550.8630	0.0097	
27.5	2536.3984	0.0039	
R_{1ff}	1.5	2404.6711	-0.0088
	2.5	2427.3204	-0.0029
	3.5	2448.4071	0.0009
	4.5	2468.1974	0.0026
	5.5	2486.7409	0.0084
	6.5	2504.0176	0.0021
	7.5	2520.0290	0.0031
	8.5	2534.7430	0.0022
9.5	2548.1338	-0.0018	

R_{2ee}

10.5	2560.1730	-0.0120
11.5	2570.8460	-0.0178
12.5	2580.1490	0.0019
13.5	2588.0110	0.0002
14.5	2594.4400	0.0090
15.5	2599.3960	0.0114
16.5	2602.8540	0.0051
17.5	2604.7980	-0.0036
18.5	2605.2220	0.0011
19.5	2604.0760	-0.0092
20.5	2601.3820	0.0089
21.5	2597.0600	-0.0029
22.5	2591.1260	-0.0070
23.5	2583.5600	-0.0012
24.5	2574.3290	0.0046
25.5	2563.3700	-0.0290
26.5	2550.7600	0.0004
27.5	2536.3819	0.0023
1.5	2429.2943	-0.0016
2.5	2449.4551	-0.0017
3.5	2468.8674	-0.0054
4.5	2487.2150	-0.0010
5.5	2504.3913	0.0088
6.5	2520.3190	0.0023
7.5	2534.9809	0.0024
8.5	2548.3370	0.0025
9.5	2560.3550	0.0006
10.5	2571.0102	0.0000
11.5	2580.2710	-0.0042
12.5	2588.1210	-0.0030
13.5	2594.5370	0.0051
14.5	2599.4780	0.0029
15.5	2602.9280	-0.0027
16.5	2604.8780	0.0020
17.5	2605.2920	0.0031
18.5	2604.1470	-0.0008
19.5	2601.4220	-0.0091
20.5	2597.1120	-0.0050

	21.5	2591.1780	-0.0058
	22.5	2583.6260	0.0168
	23.5	2574.3690	-0.0012
	24.5	2563.4030	-0.0400
	25.5	2550.8070	0.0046
	26.5	2536.4157	-0.0058
R_{2ff}	0.5	2417.3613	-0.0462
	1.5	2429.4952	-0.0021
	2.5	2449.7081	-0.0046
	3.5	2469.1862	0.0062
	4.5	2487.5717	0.0015
	5.5	-	
	6.5	2520.7620	0.0106
	7.5	2535.4536	0.0074
	8.5	2548.8321	0.0021
	9.5	2560.8710	-0.0014
	10.5	2571.5400	-0.0052
	11.5	2580.8100	-0.0117
	12.5	2588.6730	-0.0032
	13.5	2595.0880	0.0040
	14.5	2600.0240	0.0026
	15.5	2603.4730	0.0080
	16.5	2605.4020	0.0095
	17.5	2605.7740	-0.0076
	18.5	2604.6060	-0.0045
	19.5	2601.8520	-0.0057
20.5	2597.5010	-0.0004	
21.5	2591.5260	0.0062	
22.5	2583.8900	-0.0005	
23.5	2574.5950	0.0044	
24.5	2563.5940	-0.0021	
25.5	2550.8850	0.0033	
26.5	2536.4157	-0.0047	

5-4	J	ν (cm-1)	o - c
R_{1ee}	5.5	2357.8560	0.0118
	6.5	2374.1329	0.0001

	7.5	2389.1430	-0.0006
	8.5	2402.8640	0.0115
	9.5	2415.2690	0.0359
	10.5	2560.6850	-0.0053
	11.5	2435.8930	-0.0099
R_{1ff}	5.5	2357.5280	0.0017
	6.5	2373.7650	-0.0086
	7.5	2388.7680	0.0202
	8.5	2402.4230	-0.0018
	9.5	2414.7780	-0.0007
	10.5	2425.7820	-0.0008
	11.5	2435.4160	0.0054
R_{2ee}	4.5	2357.9740	-0.0264
	5.5	2374.1329	-0.0023
	6.5	2389.0290	-0.0064
	7.5	2402.6930	0.0324
	8.5	2414.9770	0.0008
	9.5	2425.9530	0.0019
	10.5	2435.5570	0.0011
R_{2ff}	5.5	2374.5040	-0.0060
	6.5	2389.4490	0.0039
	7.5	2403.1040	0.0038
	8.5	2415.4650	0.0241
	9.5	2426.4400	0.0044
	10.5	2436.0510	-0.0038